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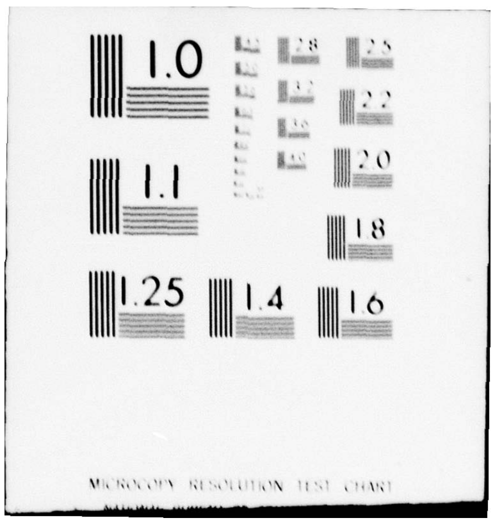
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LOCALITY PRINCIPLE IN WAVE-MECHANICS

(Wave Mechanics/Local Density of States/Local Partition Function/ Cluster Methods/Moment Methods/Path Integral Methods)

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ABSTRACT

This paper proves a locality principle for a wave-mechanical particle governed by the Schroedinger equation. It is shown that $\rho(\mathbf{r},\beta)$, the Laplace transform of the local density of states $n(\mathbf{r},E)$, depends significantly only on the potential $V(\mathbf{r}')$ at points $\mathbf{r}'$ <u>near</u> $\mathbf{r}$. The effect of changes of $V(\mathbf{r}')$ at distant points $\mathbf{r}'$ ($|\mathbf{r}' - \mathbf{r}| > d$) on $\rho(\mathbf{r},\beta)$, decay in a Gaussian fashion with a. This result sheds some light on the locality of physical properties of extended systems and provides general support for various local methods of calculation.

1. Introduction

This note deals with a particle described by the single particle Hamiltonian

$$H \equiv \frac{1}{2} p^2 + V(\mathbf{r}) \quad , \tag{1.1}$$

where $V(\mathbf{r})$ is defined for all $\mathbf{r}$ inside a large region Ω which eventually becomes infinite. The eigenfunctions and eigenvalues of H, $\psi^\nu(\mathbf{r})$ and E^ν, are defined by the Schroedinger equation

$$H\, \psi^\nu(\mathbf{r}) = E^\nu\, \psi^\nu(\mathbf{r}) \quad , \tag{1.2}$$

the boundary condition

$$\psi^\nu(\mathbf{r}) = 0 \text{ on boundary of } \Omega, \tag{1.3}$$

and the normalization condition

$$\int |\psi^\nu(\mathbf{r})|^2 \, d\mathbf{r} = 1 \; . \tag{1.4}$$

Of course a change of $V(\mathbf{r})$ in the vicinity of a point $\mathbf{r}_o$ in general changes the eigenfunctions $\psi^\nu(\mathbf{r})$ at <u>all</u> points $\mathbf{r}$. This change can be considerable even if the distance between $\mathbf{r}$ and $\mathbf{r}_o$ becomes large. For example, if we start with $V(\mathbf{r}) \equiv 0$ and Ω a large box $(-L < x,y,z < +L)$, and subsequently introduce a one dimensional localized barrier

$$V(\mathbf{r}) \equiv \begin{cases} V_o & -d < x < d \\ 0 & \text{otherwise} \end{cases} \quad , \tag{1.5}$$

the eigenfunctions $\psi^\nu(\mathbf{r})$ are changed by comparable amounts for <u>all</u> values of $\mathbf{r}$. This can be regarded as a kind of "action-at-a-distance" of the potential $V(\mathbf{r})$ on the <u>wavefunctions</u> $\psi^\nu(\mathbf{r})$.

Let us now define the quantity

$$\rho(\underset{\sim}{r},\beta) \equiv \sum_{\nu} |\psi^{\nu}(\underset{\sim}{r})|^2 \; e^{-\beta E^{\nu}} \quad , \tag{1.6}$$

which we call the local partition function (LPF). Its integral over $\underset{\sim}{r}$ is the conventional partition function,

$$Z(\beta) \equiv \int \rho(\underset{\sim}{r},\beta)d\underset{\sim}{r} = \sum_{\nu} e^{-\beta E^{\nu}} \quad . \tag{1.7}$$

Also, clearly, the LPF is the Laplace transform of the local density of states

$$n(\underset{\sim}{r},E) \equiv \sum_{\nu} |\psi^{\nu}(\underset{\sim}{r})|^2 \; \delta(E-E^{\nu}) \quad , \tag{1.8}$$

whose spatial integral is the total density of states

$$n(E) \equiv \int n(\underset{\sim}{r},E)d\underset{\sim}{r} = \sum_{\nu} \delta(E-E^{\nu}). \tag{1.9}$$

Evidently

$$\rho(\underset{\sim}{r},\beta) = \int n(\underset{\sim}{r},E) \; e^{-\beta E} \, dE \tag{1.10}$$

and

$$Z(\beta) = \int n(E) \; e^{-\beta E} \, dE \quad . \tag{1.11}$$

We shall show that, in contrast to an individual eigenfunction, $\psi^{\nu}(\underset{\sim}{r})$, the LPF $\rho(\underset{\sim}{r},\beta)$ is significantly affected by changes of $V(\underset{\sim}{r})$ only if these occur at points r_o near r. This principle, which will be made more precise below, we call locality principle of wave mechanics.

2. Proof of the Locality Principle

The proof proceeds from the path integral expression for $\rho(\underset{\sim}{r},\beta)$[1]. For convenience, we take $\underset{\sim}{r} = 0$. Then

$$\rho(\beta) \equiv \rho(0,\beta) = \int \exp\left\{-\int_0^{\beta} (\tfrac{1}{2}\, \dot{\underset{\sim}{r}}^2(u) + V(\underset{\sim}{r}))du\right\} \mathcal{D}\underset{\sim}{r}(u) \; , \tag{2.1}$$

where u is an imaginary "time" and $\mathcal{D}\underset{\sim}{r}(u)$ denotes path integration over

all paths starting and ending at $\underset{\sim}{r} = 0$.

Let us divide Ω into an interior region

$$\Omega_{int}: \qquad |x|,|y|,|z| \leqslant a \quad , \tag{2.2}$$

and an exterior region

$$\Omega_{ext}: \qquad |x|,|y|,|z| > a \quad . \tag{2.3}$$

We may then write $\rho(\beta)$ as the sum of two terms,

$$\rho(\beta) = \rho_{int}(\beta) + \rho_{ext}(\beta) \quad , \tag{2.4}$$

where $\rho_{int}(\beta)$ comprises all contributions to (2.1) coming from paths entirely inside Ω_{int}, and $\rho_{ext}(\beta)$ represents the contributions from paths extending outside Ω_{int}. We may note that $\rho_{int}(\beta)$ is the LPF for a system with potential $V(\underset{\sim}{r})$ inside Ω_{int} and infinite walls at the boundary of Ω_{int}.

Now consider a comparison potential, $V'(\underset{\sim}{r})$, identical to $V(\underset{\sim}{r})$ inside Ω_{int} but different in Ω_{ext}. The LPF for this system can be written as

$$\rho'(\beta) = \rho_{int}(\beta) + \rho'_{ext}(\beta) \quad , \tag{2.5}$$

where the interior contribution is, by the construction (2.1) the same as for $\rho(\beta)$, Eq. (2.4).

Thus the difference of the two LPFs is given by

$$\Delta\rho(\beta) \equiv \rho'(\beta) - \rho(\beta) = \rho'_{ext}(\beta) - \rho_{ext}(\beta) \quad . \tag{2.6}$$

Now let us assume that both $V(\underset{\sim}{r})$ and $V'(\underset{\sim}{r})$ are bounded below

$$V(\underset{\sim}{r}) \ , \ V'(\underset{\sim}{r}) \geqslant V_{min} \quad . \tag{2.7}$$

Then clearly, from (2.1) ,

$$\rho_{ext}(\beta),\ \ \rho'_{ext}(\beta) \leqslant \int \exp\left|-\int_0^\beta (\tfrac{1}{2}\dot{\underset{\sim}{r}}^2(u) + V_{min})du\right| \mathcal{D}_{ext}\ \underset{\sim}{r}(u)$$

$$= e^{-\beta V_{min}}\ \rho_{o,ext}(\beta)\ , \tag{2.8}$$

where $\mathcal{D}_{ext}\ \underset{\sim}{r}(u)$ denotes integration over all paths which extend into Ω_{ext} and

$$\rho_{o,ext}(\beta) \equiv \int \exp\left|-\int_0^\beta \frac{1}{2}\dot{\underset{\sim}{r}}^2(u)du\right| \mathcal{D}_{ext}\ \underset{\sim}{r}(u) \tag{2.9}$$

corresponds to a free particle, $V(\underset{\sim}{r}) \equiv 0$. Next let us assume that $V(\underset{\sim}{r})$ (but not necessarily $V'(\underset{\sim}{r})$) is bounded above,

$$V(\underset{\sim}{r}) \leqslant V_{max}\ . \tag{2.10}$$

Than clearly

$$\rho(\beta) \geqslant e^{-\beta V_{max}}\ \rho_o(\beta)\ , \tag{2.11}$$

where $\rho_o(\beta)$ is the local partition function for a free particle,

$$\rho_o(\beta) \equiv \int \exp\left| -\int_0^\beta \frac{1}{2}\dot{\underset{\sim}{r}}^2(u)du\right| \mathcal{D}\underset{\sim}{r}(u)$$

$$= \left(\frac{1}{2\pi\beta}\right)^{3/2}\ . \tag{2.12}$$

Combining Eqs. (2.6), (2.8), (2.11) and (2.12) gives

$$\frac{|\Delta\ \rho(\beta)|}{\rho(\beta)} \leqslant 2\ e^{\beta(V_{max} - V_{min})}\ \ \frac{\rho_{o,ext}(\beta)}{\rho_o(\beta)}\ . \tag{2.13}$$

Lastly we calculate $\rho_{o,ext}(\beta)$, the contribution to $\rho_o(\beta)$ of paths extending beyond Ω_{int}. We write

$$\rho_{o,ext}(\beta) = \rho_o(\beta) - \rho_{o,int}(\beta) \tag{2.14}$$

and recall that $\rho_{o,int}(\beta)$ is the LPF for free electrons in the box (2.2) with infinite walls. The cosine eigenfunctions and eigenvalues are

$$\psi^{\nu}(r) = \frac{1}{a^{3/2}} \cos\left[\frac{\pi(\nu_1+\frac{1}{2})\,x}{a}\right] \cos\left[\frac{\pi(\nu_2+\frac{1}{2})\,y}{a}\right] \cos\left[\frac{\pi(\nu_3+\frac{1}{2})\,z}{a}\right] , \tag{2.15}$$

$$E^{\nu} = \frac{1}{2}\frac{\pi^2}{a^2}\left[(\nu_1+\tfrac{1}{2})^2 + (\nu_2+\tfrac{1}{2})^2 + (\nu_3+\tfrac{1}{2})^2\right] , \tag{2.16}$$

where $\nu \equiv (\nu_1, \nu_2, \nu_3)$. Eigenfunctions which are odd in x, y or z do not contribute to the LPF at $\underset{\sim}{r} = 0$. Therefore we have

$$\rho_{o,int}(\beta) \equiv a^{-3} \sum_{\nu_1,\nu_2,\nu_3=0}^{\infty} e^{-\frac{\pi^2}{2a^2}\left[(\nu_1+\frac{1}{2})^2 + (\nu_2+\frac{1}{2})^2 + (\nu_3+\frac{1}{2})^2\right]}$$

$$= a^{-3}\left[\sum_{\mu} e^{-\beta\frac{\pi^2}{2a^2}(\mu+\frac{1}{2})^2}\right]^3 . \tag{2.17}$$

Using Poisson's summation formula[2] we can rewrite the sum over μ as

$$a^{-1}\sum_{\mu} e^{-\beta\frac{\pi^2}{2a^2}(\mu+\frac{1}{2})^2} = (2\pi\beta)^{-\frac{1}{2}}\left(1-2\sum_{n=1}^{\infty}(-1)^{n+1} e^{-\frac{2n^2a^2}{\beta}}\right) \tag{2.18}$$

so that

$$\rho_{o,ext}(\beta) = (2\pi\beta)^{-3/2}\left\{1-\left(1-2\sum_{n=1}^{\infty}(-1)^{n+1} e^{-\frac{2n^2a^2}{\beta}}\right)^3\right\} . \tag{2.19}$$

For large a only the leading term in the sum needs to be retained giving

$$\rho_{o,ext}(\beta) \to (2\pi\beta)^{-3/2}\, 6\, e^{-\frac{2a^2}{\beta}} . \tag{2.20}$$

It can be verified that the right hand side of (2.20) constitutes an upper bound on $\rho_{o,ext}(\beta)$ for <u>all</u> a,

$$\rho_{0,ext}(\beta) \leq (2\pi\beta)^{-\frac{3}{2}}\ 6\ e^{-\frac{2a^2}{\beta}} \quad . \tag{2.21}$$

Substitution of (2.12) and (2.21) into (2.13) gives our final result

$$\frac{|\Delta\rho(\beta)|}{\rho(\beta)} \leq 12\ e^{\beta(V_{max}-V_{min})}\ e^{-\frac{2a^2}{\beta}} \quad . \tag{2.22}$$

In the Appendix, a similar result is proved for the density matrix $\rho(\underset{\sim}{r},\underset{\sim}{r}';\beta)$.

3. Discussion

The key feature of Eq. (2.22) is the Gaussian decrease of $\Delta\rho(0,\beta)/\rho(0,\beta)$ with the size 2a of the cube which separates the interior and exterior regions. Thus we see that any change of the potential $V(\underset{\sim}{r})$ outside of Ω_{int}, subject only to the lower bound limitation (2.7), will have a negligible effect on $\rho(0,\beta)$, provided that a is large enough. In particular, the potential outside of Ω_{int} may be replaced by zero or Ω_{int} may be enclosed by an infinite barrier, without having an appreciable effect on $\rho(0,\beta)$.

Since $\rho(\underset{\sim}{r},\beta)$ is the Laplace transform of the local density of states $n(\underset{\sim}{r},E)$ (See Eqs. (1.8) and (1.10)) the "locality" of $\rho(\underset{\sim}{r},\beta)$ implies in a general way the locality of $n(\underset{\sim}{r},E)$. Thus the theorem (2.22) which we have derived provides a general support for the physical fact that, in an extended system physical properties near a point $\underset{\sim}{r}$ depend significantly only on the potential near $\underset{\sim}{r}$. It also lends support for various local methods of calculation, such as cluster methods[3-5], moment methods[6-7], etc., which have been extensively used in recent years to determine local properties of extended systems.

However, the Gaussian decay of $\Delta\rho(\underset{\sim}{r},\beta)$ as function of a, by no means implies that the inverse Laplace transform of $\rho(\underset{\sim}{r},\beta)$, the local density of

states $n(\underset{\sim}{r},E)$, will also be local in the same very strong sense. $n(\underset{\sim}{r},E)$ does in fact also obey a locality principle but in a much weaker sense, about which further details will be published in a contribution to the Festschrift for Felix Bloch (1979).

APPENDIX

In the following, we prove a localization theorem for the Laplace transform of the density matrix,

$$\rho(\underset{\sim}{r},\underset{\sim}{r}';\beta) \equiv \int n(\underset{\sim}{r},\underset{\sim}{r}';E)\, e^{-\beta E} dE \quad , \tag{A.1}$$

where $n(\underset{\sim}{r},\underset{\sim}{r}';E)$ is the density matrix of the system under consideration,

$$n(\underset{\sim}{r},\underset{\sim}{r}';E) = \sum_{\nu} \psi^{\nu *}(\underset{\sim}{r})\, \psi^{\nu}(\underset{\sim}{r}')\, \delta(E-E^{\nu}) \quad . \tag{A.2}$$

The Laplace transform $\rho(\underset{\sim}{r},\underset{\sim}{r}';\beta)$ can be written as a path integral similar to Eq. (2.1), where the relevant paths are those starting at $\underset{\sim}{r}$ and ending at $\underset{\sim}{r}'$. Thus, for $\underset{\sim}{r},\underset{\sim}{r}'$ inside Ω_{int}, $\rho(\underset{\sim}{r},\underset{\sim}{r}';\beta)$ obeys inequalities analogous to Eqs. (2.8) and (2.13). Consequently, in order to show that $\rho(\underset{\sim}{r},\underset{\sim}{r}';\beta)$ is localized, it suffices to show that $\rho_o(\underset{\sim}{r},\underset{\sim}{r}';\beta)$ has this property, where ρ_o is the corresponding free-electron quantity.

The contribution of paths, entirely inside the cube Ω_{int}, to ρ_o can be evaluated explicitly by using (A.1) and (A.2) and the appropriate wave functions. In this way we obtain

$$\rho_{o,int} = J(x,x')\, J(y,y')\, J(z,z') \quad , \tag{A.3}$$

where

$$J(x,x') = \sum_{n} \psi_n^*(x)\, \psi_n(x')\, e^{-\beta E_n} \quad , \tag{A.4}$$

and the set ψ_n is given by

$$\psi_{2n}(x) = a^{-\frac{1}{2}} \cos(k_{2n}x) \quad ; \quad k_{2n}a = \pi(n+\tfrac{1}{2})$$

$$\psi_{2n+1}(x) = a^{-\frac{1}{2}} \sin(k_{2n+1}a) \; ; \; k_{2n+1}a = \pi(n+1)$$

$$E_n = \tfrac{1}{2} k_n^{\,2} \quad ; \quad n = 0,\, 1,\, 2,\, \ldots \quad .$$

Separating J into even and odd contributions, and using Poisson's summation formula, one can show that

$$J = \frac{e^{-\frac{(x-x')^2}{2\beta}}}{(2\pi\beta)^{\frac{1}{2}}}\left[1 + 2\sum_{n=1}^{\infty} e^{-\frac{8a^2n^2}{\beta}} \cosh\left[\frac{4an(x-x')}{\beta}\right] - 2\, e^{-\frac{2xx'}{\beta}} \sum_{n=1}^{\infty} e^{-\frac{2a^2(2n-1)^2}{\beta}} \cosh\left[\frac{2a(2n-1)(x+x')}{\beta}\right]\right] \tag{A.5}$$

For a large cube of edge 2a, and for x and x' close enough to the origin (in such a way that $|x| + |x'| \ll a$), the series in (A.5) converge very rapidly and can be replaced by the corresponding first terms. In this way we obtain

$$J(x,x') = J_\infty(x,x')\left\{1 + 2e^{-\frac{8a^2}{\beta}} \cosh\left[\frac{4a(x-x')}{\beta}\right] - 2e^{-\frac{2(a^2+xx')}{\beta}} \cosh\left[\frac{2a(x+x')}{\beta}\right]\right\} \tag{A.6}$$

where J_∞ is the corresponding contribution from an infinite system, i.e.,

$$J_\infty(x,x') = (2\pi\beta)^{-\frac{1}{2}}\, e^{-\frac{(x-x')^2}{2\beta}} \tag{A.7}$$

We apply now Eqs. (2.13), (A.3) and (A.8) to obtain the following localization theorem:

$$\frac{|\Delta\rho(\underset{\sim}{r},\underset{\sim}{r}';\beta)|}{\rho(\underset{\sim}{r};\underset{\sim}{r}';\beta)} \leq 2e^{\beta(V_{max}-V_{min})}\left[1 - g(x,x')\, g(y,y')\, g(z,z')\right] , \tag{A.8}$$

where $\Delta\rho$ is the change in ρ due to the change in the potential outside of Ω_{int}, and g is given by

$$g(x,x') = 1 - 2e^{-\frac{2a^2}{\beta}}\left\{e^{-\frac{2xx'}{\beta}}\cosh\left[\frac{2a(x+x')}{\beta}\right] - e^{-\frac{6a^2}{\beta}}\cosh\left[\frac{4a(x-x')}{\beta}\right]\right\} \tag{A.9}$$

We note that the relation (2.22) is a particular case of the general result (A.8) with $\underset{\sim}{r} = \underset{\sim}{r}' = 0$.

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